Triisopropanolamine

122-20-3 | DTXSID5021415

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 25.4 L/kg

Global applicability domain: Inside

Local applicability domain index: 3.81e-01

Confidence level: 6.44e-01

Nearest Neighbors from the Training Set

Image not found
Oxamyl
Measured: 10.0
Predicted: 15.0

Image not found
Daminozide
Measured: 8.91
Predicted: 10.9

Image not found
Uracil mustard
Measured: 28.8
Predicted: 37.5

Image not found
Propamocarb hydrochloride
Measured: 309
Predicted: 218

Image not found
Allidochlor
Measured: 20.0
Predicted: 24.7